AN ANALYSIS OF THE ν_3 BAND OF HTO AIDED BY THE PARTRIDGE AND SCHWENKE POTENTIAL ENERGY SURFACE

M. TINE AND L. H. COUDERT, *LISA, CNRS/Universités Paris 12 et 7, 61 Avenue du Général de Gaulle, 94010 Créteil, France*.

Although the HTO molecule is an unstable species containing a radioactive tritium atom, its high-resolution spectrum have already been the subject of several investigations. In the seventies, Helminger *et al.*[a] were able to measure 41 transitions in its microwave spectrum. Later, Cope *et al.*[b] studied the fundamental ν_1 band, corresponding to the OT stretching mode. The high-resolution spectrum of the ν_3 fundamental band, which corresponds to the OH stretching mode, was recorded in the early seventies by Guy Steinbeckeliers and André Fayt using a grating spectrometer. However, the analysis of this spectrum was never carried out.

In this paper the analysis of this high-resolution spectrum will be presented. The spectrum assignment will be described and the results of a preliminary analysis of the line positions, carried out using a Watson-type Hamiltonian, will be reported. This preliminary analysis was not satisfactory as some infrared transitions displayed observed minus calculated differences much larger than the experimental uncertainty on their observed wavenumbers. This, in addition to the fact that the distortion constants for the (001) state had too large values, clearly indicates that this state is perturbed. The perturbing state is likely to be the (110) state for which no spectroscopic data are available.

In order to obtain spectroscopic informations on the perturbing state, a calculation of its rotational energy levels was undertaken using the tridimensionnal potential energy surface published by Partridge and Schwenke.[c] Work is still in progress and we are hoping to be able to calculate more accurately the energy of the (001) state using a model in which this state and the (110) states are treated together.

---

[a] P. Helminger, F. C. De Lucia, W. Gordy, P. Staats, and H. W. Morgan, *Phys. Rev. A* **10,** 1072 (1974).

[b] S. D. Cope, D K. Russel, H. A. Fry, L. H. Jones, and J. E. Barefield, *J. Molec. Spectrosc.* **127,** 464 (1988).

[c] H. Partridge and D. W. Schwenke, *J. Chem. Phys.* **106,** 4618 (1997).